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Advanced Scientific Computing Research

Large Scale Production Computing Requirements Workshop for Biological and Environmental Research

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Outline of Introduction

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- Current approaches to NERSC requirements gathering
- Benefits of SC/HQ-centric requirements gathering for NERSC resources in the context of Programmatic mission needs
- SC/ASCR HPC Facilities and their missions
- NERSC roles in SC HPC services
- Purpose of this workshop

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Current Tools for Requirements Gathering for NERSC

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Document or Action	Owner/Perspective	Frequency
DOE Greenbook – Needs and Directions in High-Performance Computing for the Office of Science, June 2005	NERSC User Group (NUG)/NERSC users	Once every three - five years
NERSC "Visualization Greenbook," October 2002	NUG/NERSC users	Not set
Science-Driven Computing: NERSC's Plan for 2006-2010, May 2005	LBNL NERSC/LBNL NERSC	Once every five years

Assessment of Current Tools

- These documents are very informative.
- They represent either NERSC's User Group's perspective, or LBNL/NERSC Team's perspective.
- *Science-Driven Computing: NERSC's Plan* is the closest to capture SC's needs, and is published once every 5 years.
- Science needs are changing rapidly, and the five-year cycle does not capture the changing needs very effectively.
- We also need more computation-oriented data for NERSC needs than those currently collected using the existing mechanisms.

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Benefits of Conducting NERSC Requirements Workshops in Three-Year Cycle

- SC Program Offices will have direct input on and validation of the requirements and can provide forecasts of needs aligned with mission priorities.
- Requirements gathering workshops in the DC area in the three-year cycle can capture rapidly changing Program-specific needs for NERSC resources better.
- We can document SC programmatic needs for NERSC resources that may not be captured in the five-year cycle planning tools.
- We can leverage the successful structure and approach used for the ESnet requirements workshops.

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ASCR HEC Facilities: Providing the Tools

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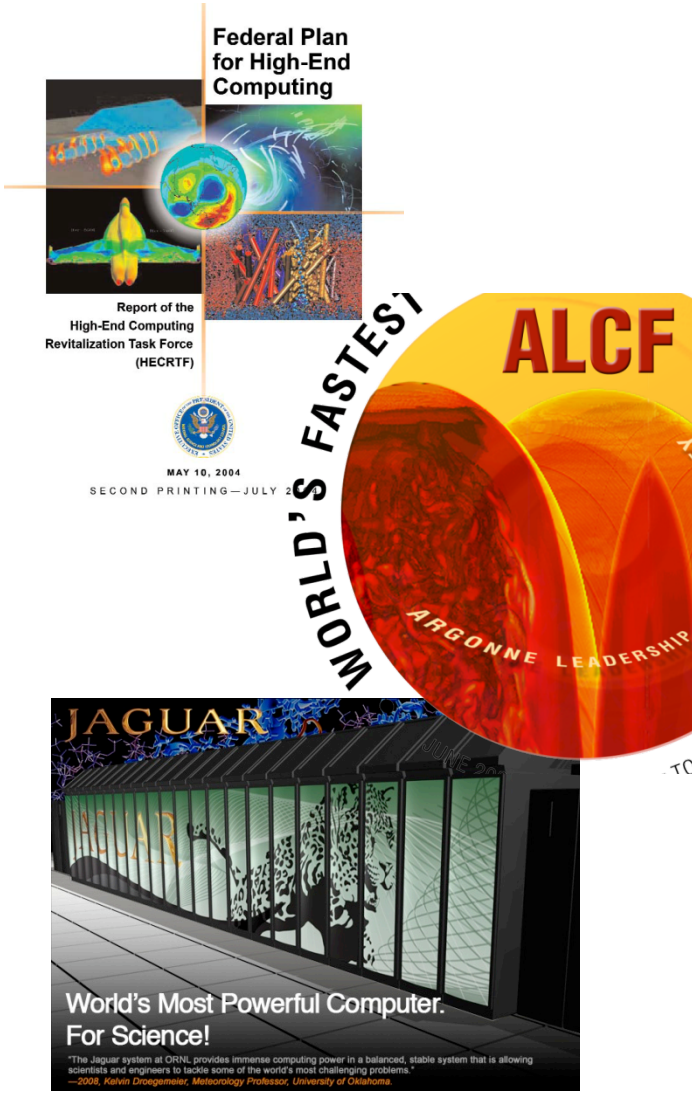
- High-Performance Production Computing - National Energy Research Scientific Computing Center **(NERSC)** at Lawrence Berkeley National Laboratory
  - Delivers high-end computing to entire DOE SC research community to make world-class scientific discovery
  - Facilitates the improved scalability of applications that will enable them to compete for time at a Leadership Class Facility (LCF)
- Leadership-Class Computing – **Leadership Computing Centers at Argonne National Laboratory and Oak Ridge National Laboratory**
  - Delivers highest computational capability to national and international researchers through peer-reviewed **Innovative and Novel Computational Impact on Theory and Computation (INCITE)** program (80% of resources)



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NERSC Role in ASCR HPC: Keystone

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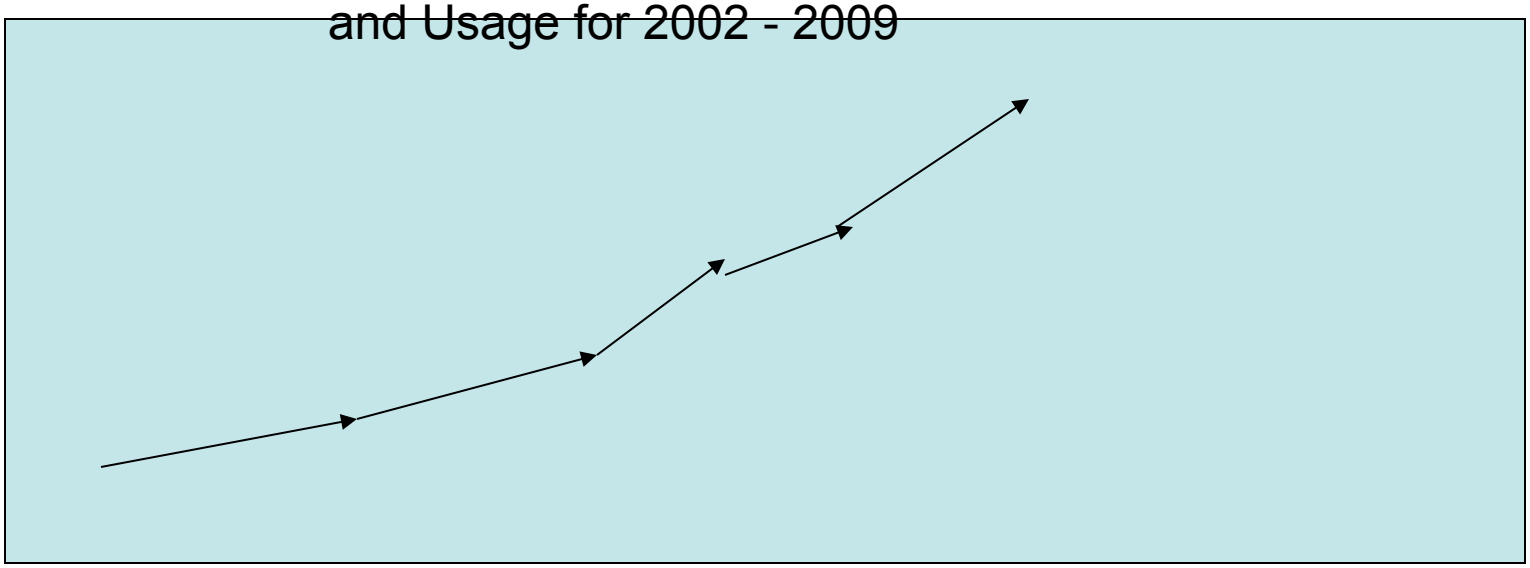
- "NERSC continues to be a gold standard of a scientific High Performance Computational facility." – HPCOA Review August 2008
- Introduction of INCITE and LCFs has not reduced needs for NERSC services.

Include a graph showing Hors Requested and Usage for 2002 - 2009



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Purpose of This Workshop

- The goal of this workshop is to accurately characterize the High Performance Computing (HPC) requirements of current and future work funded by the Office of Biological and Environmental Research (BER).
- These requirements will serve as input to the NERSC architecture and planning processes, and will help ensure that NERSC continues to provide world-class support for scientific discovery for DOE scientists and their collaborators.
- The tangible outcome of the workshop will be a document that includes both HPC requirements and a supporting narrative.